Finite-Size Scaling and Damage Spreading in Ising Systems with Multispin Interactions

Ubiraci P. C. Neves and J. R. Drugowich de Felício

Departamento de Física e Matemática, FFCLRP, Universidade de São Paulo
Av. Bandeirantes, 3900 - CEP: 14040-901 - Rib. Preto, SP, Brazil

Abstract

We investigate two-dimensional Ising systems with multisping interactions of three- ($m = 3$) and four-body terms ($m = 4$). The application of a new type of finite-size algorithm of de Oliveira allow us to clearly distinguish a first-order transition (in the $m = 4$ case) from a continuous one (in the $m = 3$ one). We also study the damage spreading in these systems. In this study, a dynamical phenomenon is observed to occur at a critical point separating a chaotic phase from a frozen one. However, the width of the interval where this transition happens does not yield a conclusive evidence about the order of the phase transition.

1 Introduction

The presence of multispin interactions can lead to severe alterations in the behavior of statistical mechanical models such as the Baxter and the Ashkin-Teller models. There are other models of the same type and these can include three-, four- or more-body terms in dimension $d \geq 2$. For instance, we may cite the Ising system with multispin interactions. For a two-dimensional problem, the Hamiltonian H of such an Ising-like system is expressed by

$$-\frac{1}{k_B T}\, H = \sum_{\langle ij \rangle} \left\{ K_y\, S_{i,j}\, S_{i+1,j} \,+\, K_x \prod_{l=0}^{m-1} S_{i,j+l} \right\} , \qquad (1)$$

where k_B is the Boltzmann constant, T is the temperature and $S_{i,j} = \pm 1$ is a boolean variable localized on site (i, j).

Turban and Debierre [1] have looked at this anisotropic model and shown that it has a single transition located at the self-dual critical point, once the above Hamiltonian is self-dual for any m. The critical point can be determined through the known relation $\sinh(2K_x)\sinh(2K_y) = 1$, which is independent of m. For the isotropic case ($K_x = K_y$), the physical solution of this relation is $K_x = K_y = K_c = \frac{1}{2}\ln(1+\sqrt{2}) = 0.44068679...$. From the spin reversal invariance of the Hamiltonian as well as from an analysis of the energy of domain walls, one can see that the ground state is 2^{m-1} times degenerate and expect that the model will be on the same universality class as the q-state Potts model whenever $q = 2^{m-1}$ [1,2].

Mean-field theory [1] and finite size scaling [1,3-6] were first used to study this problem. Further improvements of the mean-field methods [7] and Monte Carlo simulations [8] helped to indicate a first-order transition in the $m = 4$ case. The method of the fourth-order cumulant of Challa, Landau and Binder [9] and a Monte Carlo histogram technique of Ferrenberg and Swendsen [10] were then used to study the order of the transitions in the $m = 3$ and $m = 4$ cases [2]: the phase transition was characterized to be continuous in the $m = 3$ case and was asserted to be a first-order one in the $m = 4$ case.

In the present study, we apply a new type of finite-size scaling algorithm [11] to study the critical properties of the above model. We clearly distinguish a first-order transition (in the $m = 4$ case) from a continuous one (in the $m = 3$ case). In addition, we obtain good collapsed curves when the pertinent exponents are used.

We also consider the dynamics of *spreading phenomena* [12,13] in the system. A critical parameter K_d which separates a chaotic phase from a frozen one is obtained in both cases ($m = 3$ and $m = 4$). However, unlike the finite-size scaling method, a *damage spreading* analysis [14-16] seems to

be *not* able to characterize the order of the phase transition.

2 Finite-Size Scaling

The finite-size scaling algorithm of de Oliveira [11,17] is based on two thermodynamic quantities, namely the bulk quantity Q and the surface correlation function τ.

For an Ising system, τ can be calculated as follows: one considers two opposite surfaces of the lattice and verifies which spin state dominates each one of them. A counter is increased by 1 if both surfaces are dominated by the same state, otherwise it is decreased by 1. This counter is normalized by the number of measurements and the result is denoted by τ. In this way, τ is a step function of $T - T_c$. For $T < T_c$ the surfaces are well-correlated and $\tau = 1$, whereas for $T > T_c$ the surfaces are uncorrelated and thus $\tau = 0$. This criterion holds for second-order transitions where the correlation length diverges; however, at a first-order transition the correlation length remains finite and thus a multidomain state is possible even below T_c, which implies that this normalized counter may be close to zero in some samples and close to 1 in other samples [17].

The bulk quantity Q is the average of the *sign* of the sum of the Ising spins ± 1 [11,18].

Both quantities Q and τ are shown [11,18] to scale as L^0 at the critical temperature T_c and in the thermodynamic limit (L is the linear size of the system). So they behave like Binder's fourth-order cumulant [19].The function Q is based on a bulk measure of the majority of spins, whereas τ measures the correlation between two opposite surfaces of the system [17].

Another important quantity is the *bulk magnetization* M. For an Ising system, it is the average of the absolute value of the sum of all spins [11]. At the critical temperature, this quantity scales as $M \sim L^y$, where y is the magnetic exponent. For a continuous phase transition, the exponent is $y = D - \frac{\beta}{\nu}$, where D is the geometrical dimension of the system, β is the exponent associated to the spontaneous magnetization (order parameter) and ν is the thermal critical exponent which governs the divergence of the correlation length. The definition of y can be extended even to a first-order transition, where the exponent ν cannot be defined. In this case, $M \sim L^D$ and thus $y = D$ [17].

We simulate two-dimensional Ising systems with multispin interactions and Hamiltonian expressed by (1) for the cases $m = 3$ and $m = 4$. For each Monte Carlo updating, spins are selected sequentially and flipped with the thermal probability of the Metropolis algorithm. Simulations are performed

on the square lattice with periodic boundary conditions for different lattice sizes L. For fixed K_x $(= K_y)$, we average the quantities τ and M over a total of $(2-4)\times 10^5$ Monte Carlo steps after discarding the initial 4×10^4 transient steps. In order to obtain these averages, we consider a subset of spins belonging to the rows of sites which are separated from each other by multiples of m lattice parameters. In this way, we may calculate the magnetization as the average of the modulus of m times the sum of all spins belonging to those rows. The surface correlation function may be calculated as defined above provided that the two mentioned opposite surfaces correspond to two of those rows which are $L/2$ lattice parameters apart from each other. The statistics is improved by averaging over all possible subsets of rows of sites.

The bulk magnetization M is measured at K_c for different linear sizes L. The plots of M versus L in logarithmic scale are presented in Figure 1 (for simulations with $m = 3$) and in Figure 2 (for $m = 4$). The straight lines confirm the scaling relation $M \sim L^y$. For $m = 3$, the magnetic exponent obtained is $y = 1.83 \pm 0.03$. This result is really consistent with the expected *second-order* value $y = D - \frac{\beta}{\nu} = 2 - \frac{3}{16} = 1.8125$ (this model is considered to be on the same universality class as the $q = 4$ Potts and Baxter-Wu [20] models with exponents $\alpha = \nu = 2/3$ but $\beta = 1/8$ [7]). For $m = 4$, we obtain the value $y = 2.08 \pm 0.05$ which points to the expected *first-order* transition with magnetic exponent $y = D = 2$ (remind that the $m = 4$ case should be on the same universality class as the $q = 8$ Potts model). So this finite-size scaling method seems to be still very trustworthy when applied to Ising systems with multispin interactions. It is a way to provide a clear determination of a first-order phase transition as well as a second-order one.

Figure 1 to be inserted here.

Figure 2 to be inserted here.

Additionally, plots of the surface correlation function τ versus $L^{1/\nu}$ $(K_x - K_c)$ for different sizes L can lead to estimatives of the critical coupling K_c

and the thermal exponent ν by adjusting these parameters so that all points collapse onto the same curve [17]. We instead prefer to show that we do obtain this collapse if the known values of K_c and ν are previously used. Data from simulations with $m = 3$ lead to the plot of τ versus $L^{1/\nu}\ (K_x - K_c)$ (with $\nu = 2/3$) as shown in Figure 3. In this graph, the points correspond to discrete values of K_x nearby K_c for lattice sizes $L = 30$ (+), 60 ($\star$) and 90 ($\boxdot$). A good collapse is observed for all three sets of points. In the case $m = 4$ where the thermal exponent ν is not defined we can also obtain a collapse if we consider the artificial value $\nu = 1/2$. In Figure 4, we thus plot τ versus $L^2\ (K_x - K_c)$ for $m = 4$ and lattice sizes $L = 32$ (+), 64 ($\star$) and 96 ($\boxdot$). One should consider the standard deviations $\Delta\tau$ of some points when appreciating the accuracy of the collapse: in our simulations statistical errors may reach the value $\Delta\tau \sim 0.1$ for those points on the fall of curve corresponding to $L = 96$ ($\boxdot$).

Figure 3 to be inserted here.

Figure 4 to be inserted here.

3 Damage Spreading

Of late years the damage spreading method has been used as a numerical approach to study the propagation of a perturbation throughout many systems such as spin glasses [12], Ising model [13-15], q-state Potts model [16] and cellular automata [21]. In the present work, we study damage spreading in Ising systems with multispin interactions. We again investigate the Ising-like system (on the square lattice) with a Hamiltonian described by equation (1) with $K_y = K_x$. Consider that the time evolution of two independent spin configurations of the system is governed by the same dynamics and the same

sequence of random numbers generated in the Monte Carlo process. Let $A_t = \{S^A_{i,j}(t)\}$ and $B_t = \{S^B_{i,j}(t)\}$ be these two configurations at time t. The *total damage* $D(t)$ between them is defined as the fraction of corresponding spins with different signs, that is,

$$D(t) = \frac{1}{2N} \sum_{i,j} |S^A_{i,j}(t) - S^B_{i,j}(t)| \,, \tag{2}$$

where N is the number of lattice sites.

A starting configuration is thermalized at a fixed K_x ($\propto 1/T$) by the Glauber dynamics. At time $t = 0$, this thermalized configuration is termed A_0 and a second configuration B_0 is created from A_0 by flipping ("damaging") a chosen fraction $D(0) = M/N$ of corresponding spins. Then both configurations evolve in time according to this same dynamics and with the same sequence of random numbers. After a transient (2000 steps per site), we get a time average of $D(t)$ (over 7000 Monte Carlo steps). We calculate its medium value $< D(t) >$ over several samples of configurations A_0 and B_0, for each K_x and initial damage $D(0)$. From a total of 50 initial samples, we only average over those configurations where damage is non null (unless all of them present a damage that has become equal to zero).

In a Monte Carlo step at time t, all lattice sites (i, j) are sequentially visited and each spin $S_{i,j}(t)$ is flipped with probability

$$p_{i,j}(t) = \frac{1}{1 + \exp(\frac{\triangle H}{k_B T})} \tag{3}$$

where $\triangle H$ is energy change associated with such a possible spin-flip. The numerical procedure for updating the spins consists in generating a sequence of random numbers $r_{i,j}(t)$ uniformly distributed in the interval $[0, 1]$ and setting $S_{i,j}(t+1) = -S_{i,j}(t)$ if $r_{i,j}(t) \leq p_{i,j}(t)$ or setting $S_{i,j}(t+1) = S_{i,j}(t)$ otherwise. One must use the same sequence $r_{i,j}(t)$ for updating both configurations A_t and B_t.

We simulate Ising-like systems on square lattices $L \times L$ with periodic boundary conditions. The averaged long-time damage $< D(t) >$ versus K_x for the case $m = 3$ (with $L = 42$) is presented in Figure 5 whereas results corresponding to $m = 4$ (with $L = 40$) are shown in Figure 6. For each case we plot two curves: one of them connects the points (squares) obtained from simulations with initial damage $D(0) = 1/N = 1/L^2$ and the other one (star points) corresponds to $D(0) = 0.90$.

Figure 5 to be inserted here.

Figure 6 to be inserted here.

In both graphs, for the lower values of K_x (corresponding to the higher temperatures) the long-time damage reaches the value $D^* = 1/2$ which is the same result from Glauber dynamics for damage spreading in the Ising Model. In fact, there are also two states per spin in the multispin Ising system so two corresponding spins $S^A_{i,j}(t)$ and $S^B_{i,j}(t)$ present 4 possible configurations. For those values of K_x, all 4 possibilities should be equally probable but only half of them would correspond to damaged configurations. So there is a range of low values of K_x where the damage does not depend on the initial conditions. However, exactly at $K_x = 0$, one should note $p_{i,j}(t) = 1/2$ so that two corresponding spins would (or would not) simultaneously change their states thus preserving the initial damage ($< D(t) >= D(0)$). There is also another situation where the initial damage is preserved: for $D(0) = 1$ and $m = 4$ one can easily prove that two corresponding spins have the same probability $p_{i,j}(t)$ of flipping (the preservation of initial damage $D(0) = 1$ has been already observed for the $m = 2$ Ising ferromagnet).

For higher values of K_x (or lower temperatures) the damage depends on the initial conditions. In this case, we observe that if the initial damage is $D(0) < 1/2$ then the long-time damage is $< D(t) >= 0$ for both $m = 3$ and $m = 4$. On the other hand, if $D(0) > 1/2$ then $< D(t) >\rightarrow 2/3$ for $m = 3$ whereas $< D(t) >\rightarrow 1$ for $m = 4$. This behaviour is illustrated in Figures 5 and 6 for the chosen values $D(0) = 1/L^2 < 1/2$ and $D(0) = 0.90 > 1/2$.

For increasing K_x close to K_c the damage changes from $D^* = 1/2$ to the value corresponding to the second plateau of each curve. Oscillations in the critical region are due to statistical fluctuations. The standard deviations of those points in the critical interval may vary from ~ 0.05 unit (star points) up to ~ 0.15 (squares).

Similar dynamical critical phenomenon has been already observed in the literature for Ising [15] and q-state Potts models (with Hamiltonian given by

$H = -J \sum_{<ij>} \delta(\sigma_i, \sigma_j))$ [16]. In reference [16], it has been shown that simulations of damage spreading in the q-state Potts model through a Glauber dynamics yielded a frozen phase for a temperature $T < T_d$ and a chaotic phase for $T \geq T_d$. Damage was observed to assume a high-temperature value $(q-1)/q$ above a characteristic temperature $T^* \geq T_d$. This allowed the authors to define an interval $\triangle T = T^* - T_d$ whose q dependence presented a decreasing behaviour with increasing values of q, giving "some indication of the order of the phase transition" [16].

The above fact has motivated us to investigate the order of the phase transiton in the $m = 3$ and $m = 4$ multispin Ising systems through a damage spreading analysis. Our results above (expressed as functions of the coupling K_x instead of T) show that, in fact, there is a dynamical critical phenomenon at a critical coupling K_d so that for $K_x \leq K_d$ the damage is insensitive to its initial value (*chaotic phase*) whereas for $K_x > K_d$ there are two definite constant values of damage corresponding to initial conditions $D(0) < 1/2$ and $D(0) > 1/2$ (*frozen phase*). We estimate $K_d = 0.440(1)$ for $m = 3$ (Figure 5) and $K_d = 0.444(1)$ for $m = 4$ (Figure 6). We also identify a characteristic coupling $K^* \leq K_d$ so that for $K_x \leq K^*$ the damage assumes the value $D^* = 1/2$ and the curves corresponding to different initial conditions join themselves. Then we estimate an interval $\Delta K = K_d - K^* = 0.006(2)$ for $m = 3$ and $\Delta K = 0.008(2)$ for $m = 4$. The first result might be compared with the interval $\Delta K \sim \frac{J}{2k_B}\left(\frac{1}{T_d} - \frac{1}{T^*}\right) \sim \frac{1}{2}\left(\frac{1}{0.90} - \frac{1}{0.91}\right) \sim 0.006$ (for the $q = 4$ Potts model) extracted from Fig. 3 of reference [16], where the *non vanishing* interval was taken as an indicator of the continuous phase transition. On the other hand, the estimative of the interval ΔK for $m = 4$ *does not* allow us to characterize the order of the phase transition (which is discontinuous in this case).

4 Conclusion

In summary, in order to investigate the phase transition of Ising systems with multispin interactions we have applied two methods: a finite-size scaling algorithm of de Oliveira [11] and a damage spreading analysis.

Through the finite-size scaling method we have obtained the scaling relation for bulk magnetization, $M \sim L^y$, with magnetic exponents consistent with the expected second-order transition value $y = 1.8125$ (for $m = 3$) and first-order transition value $y = D = 2$ (for $m = 4$). In this way the orders of phase transitions in the $m = 3$ and $m = 4$ multispin Ising systems have been clearly distinguished. Additionally, plots of the surface correlation function τ versus $L^{1/\nu}(K_x - K_c)$ for different sizes L have collapsed onto the same

curve, showing that this technique can also be used as a way to estimate K_c and ν.

Regarding the analysis of damage spreading in the system, we have observed a dynamical critical phenomenon at a critical coupling $K_d \approx K_c$ separating a chaotic phase (where damage is insensitive to its initial value) from a frozen phase (with two definite constant values of damage). However, the width ΔK of the interval where this transition occurs has not yielded a conclusive evidence about the order of the phase transition.

Acknowledgments

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FIGURES CAPTION

Figure 1 - Bulk magnetization M at K_c from simulations with $m = 3$ for linear lattice sizes $L = 30,\ 42,\ 54,\ 66,\ 78,\ 90\ , 120$ and 150. The straight line confirms the scaling relation $M \sim L^y$ with magnetic exponent $y = 1.83 \pm 0.03$ which is consistent with the value $y = D - \frac{\beta}{\nu} = 1.8125$ expected for a second-order transition.

Figure 2 - Bulk magnetization M at K_c from simulations with $m = 4$ for linear lattice sizes $L = 32,\ 48,\ 64,\ 80,\ 96,\ 112\ , 128$ and 144. The straight line confirms the scaling relation $M \sim L^y$ with magnetic exponent $y = 2.08 \pm 0.05$ pointing to the expected first-order transition value $y = D = 2$.

Figure 3 - Plot of the surface correlation function τ versus $L^{1/\nu}\ (K_x - K_c)$ (with $\nu = 2/3$) for $m = 3$ and lattice sizes $L = 30$ (+), 60 ($\star$) and 90 ($\boxdot$).

Figure 4 - Plot of the surface correlation function τ versus $L^2\ (K_x - K_c)$ for $m = 4$ and lattice sizes $L = 32$ (+), 64 ($\star$) and 96 ($\boxdot$).

Figure 5 - Average damage $< D(t) >$ versus K_x for the $m = 3$ multispin Ising system with $L = 42$. The squares ($\boxdot$) represent points obtained from simulations with initial damage $D(0) = 1/N = 1/L^2 < 1/2$ and the star points ($\star$) correspond to $D(0) = 0.90 > 1/2$.

Figure 6 - Average damage $< D(t) >$ versus K_x for the $m = 4$ multispin Ising system with $L = 40$. The squares ($\boxdot$) represent points obtained from simulations with initial damage $D(0) = 1/N = 1/L^2 < 1/2$ and the star points ($\star$) correspond to $D(0) = 0.90 > 1/2$.

FIGURE 1

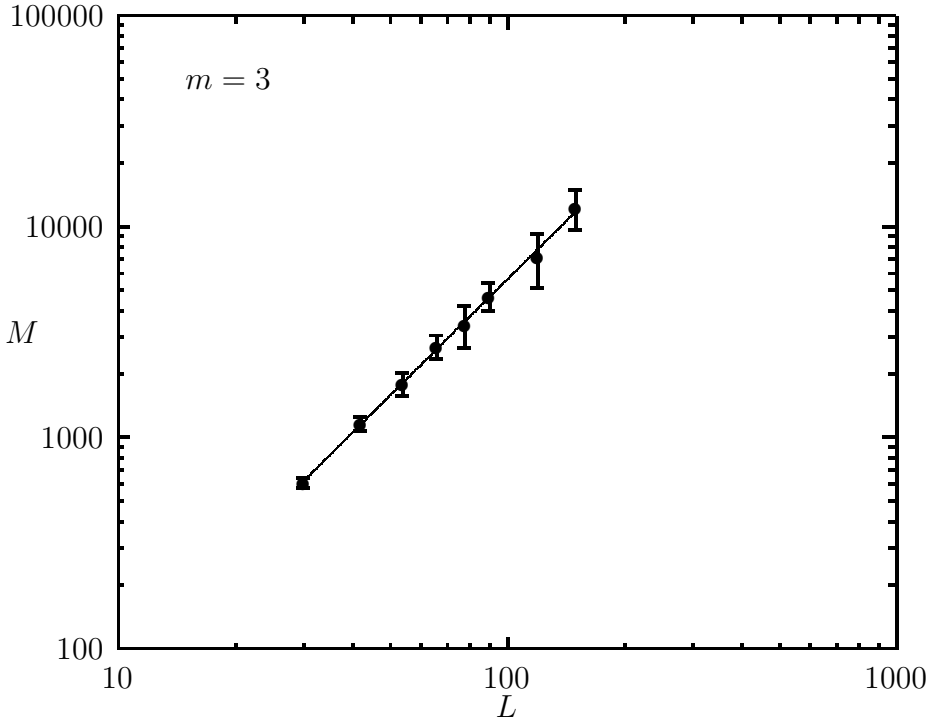


FIGURE 2

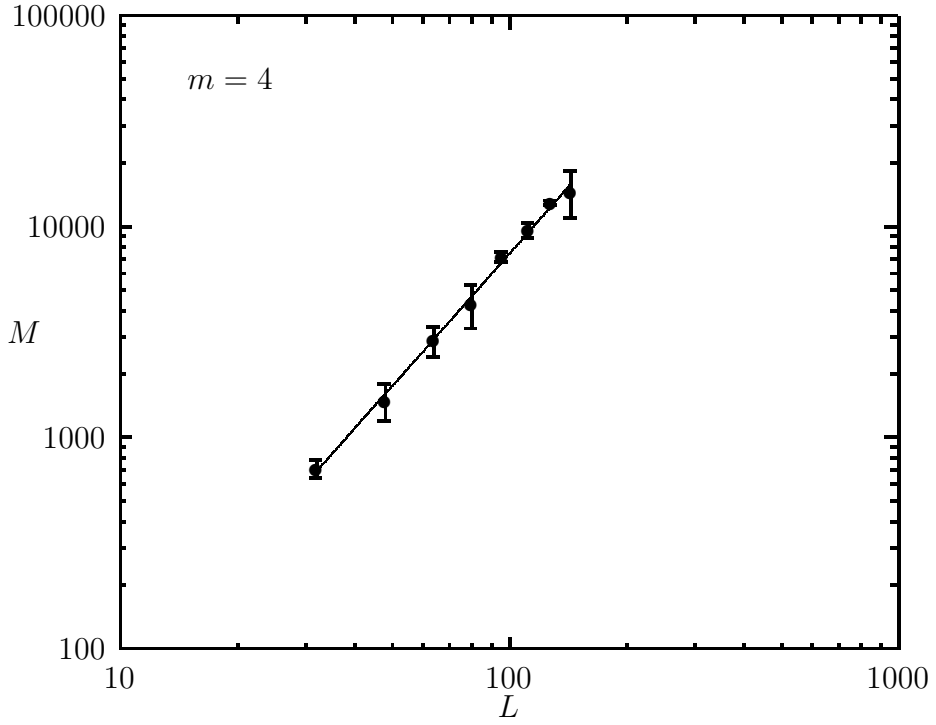


FIGURE 3

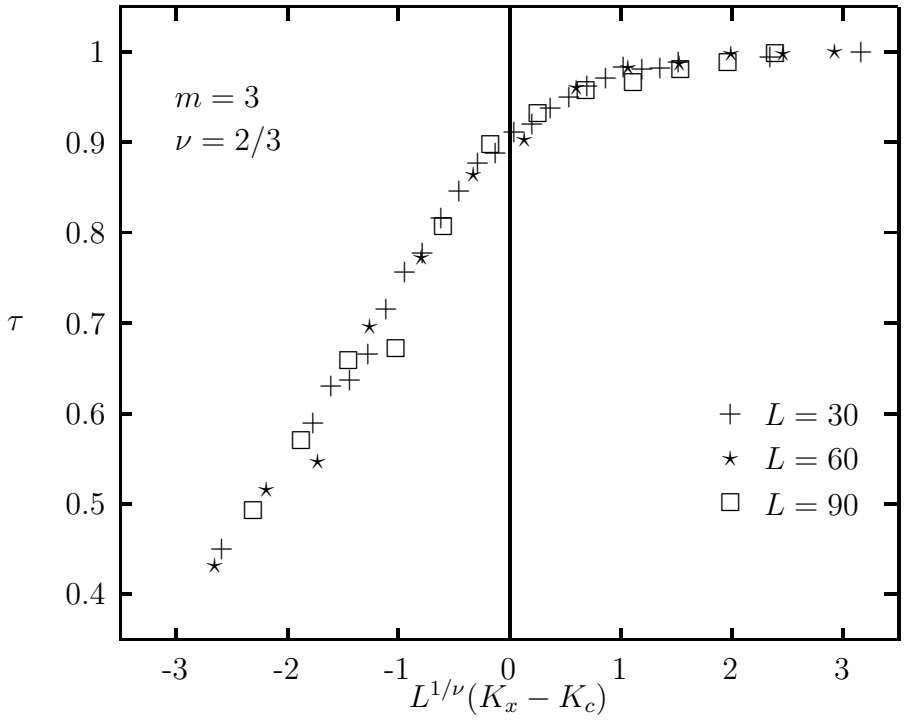
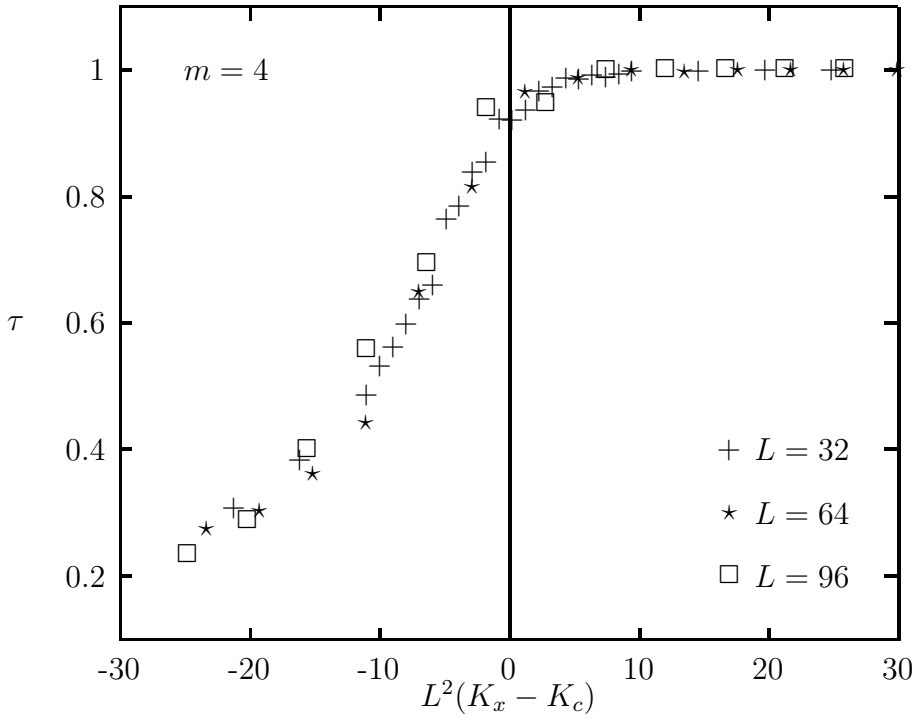


FIGURE 4


$m = 4$
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0.8
0.6
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-30
-20
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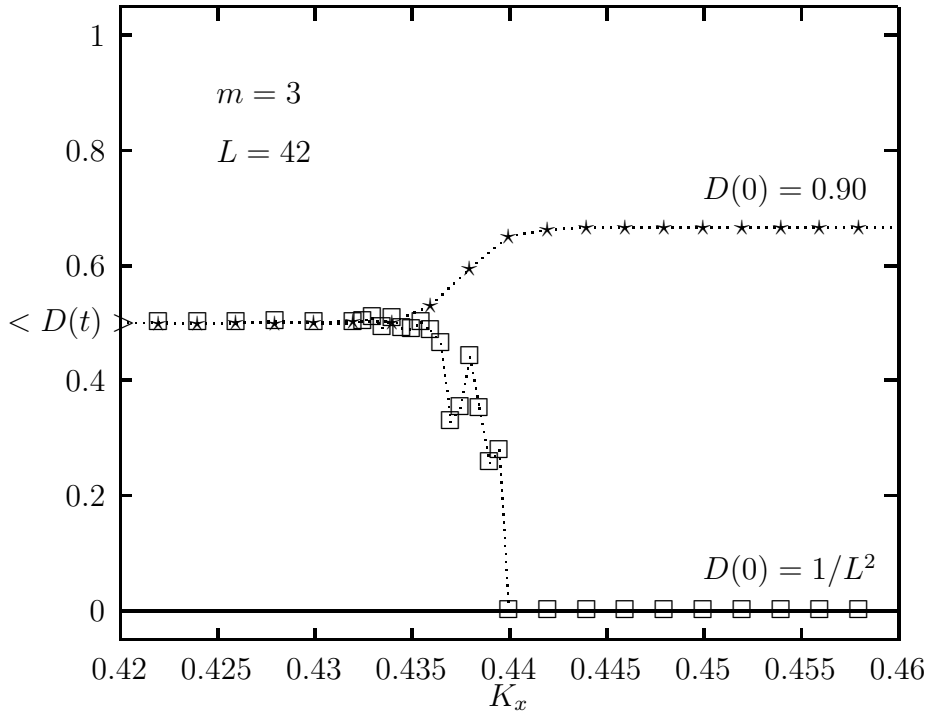
$\star$ $L = 64$
$\square$ $L = 96$

FIGURE 5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$D(0) = 0.90$
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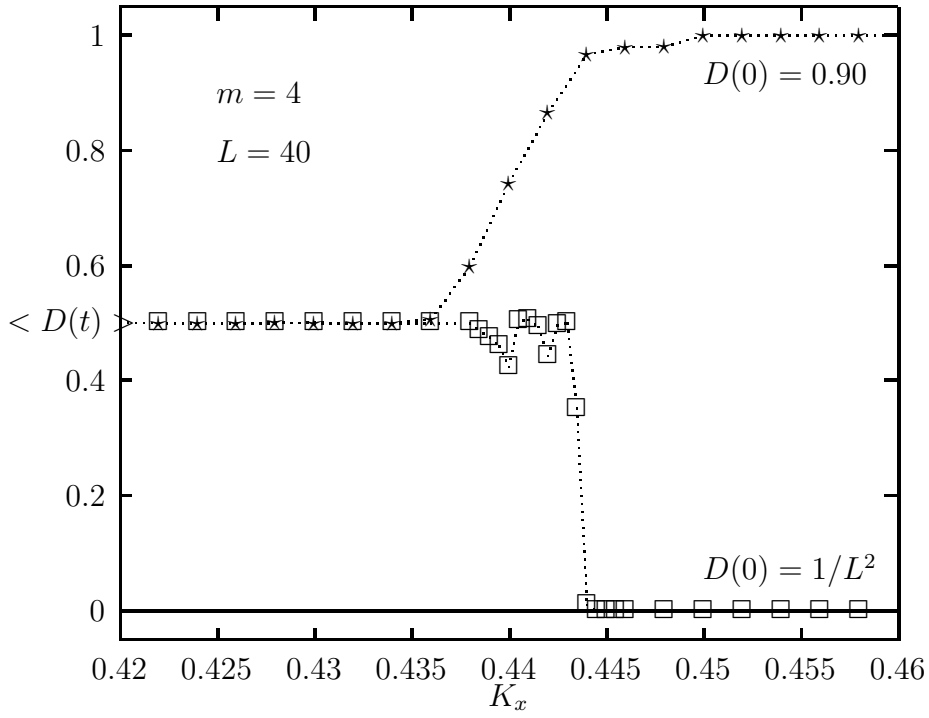
K_x

FIGURE 6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